



chain nodes :

7 8 9 10 17

ring nodes :

1 2 3 4 5 6 11 12 13 14 15 16 20 21 22 23 24 25

chain bonds :

3-24 6-8 7-21 8-9 8-10 10-13

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 20-21 20-25 21-22
22-23 23-24 24-25

exact/norm bonds :

7-21 8-9 8-10 10-13

exact bonds :

3-24 6-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16 20-21 20-25 21-22
22-23 23-24 24-25

isolated ring systems :

containing 1 : 11 : 20 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:Atom 20:Atom 21:CLASS 22:Atom
23:Atom 24:Atom 25:Atom